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# The formulation of quantum mechanics in terms of phase space functions—the third equation

David B Fairlie† and Corinne A Manogue‡§

† Department of Mathematical Sciences University of Durham, Durham DH1 3LE, UK

‡ Department of Physics Oregon State University, Corvallis, OR 97331, USA

§ Mathematical Sciences Research Institute 1000 Centennial Drive, Berkeley, CA 94720, USA

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**Abstract.** The formalism of the Wigner distribution function is reviewed. In addition to the Liouville equation, which expresses the time rate of change of this function in terms of its Moyal bracket with the Hamiltonian, and its expression as a projection operator, a third equation is proposed with the aid of an auxiliary variable  $s$ , to which a formal solution is constructed in terms of known quantum-mechanical eigenfunctions and eigenvalues. In addition, an *ab initio* solution to the three equations in terms of an error function is found for the free particle in one dimension. Two views are advanced: the orthodox, that this new equation is merely a consistency requirement, and the speculative, that the measurement process has something to do with the choice of  $s$ .

## 1. The Wigner distribution function

There are many presentations of quantum mechanics of which the best known are the original Schrödinger-Dirac-Heisenberg formulation, and the functional integral approach of Feynman. There is a third, the phase space formulation of quantum mechanics due to Wigner [1], which is much less well known, but which has enjoyed something of a revival recently in the context of quantum optics. Wigner wanted to construct an object from the quantum-mechanical wave function which behaved like a conventional probability distribution; he succeeded in constructing a distribution which was real, but not positive. Moyal then wrote the evolution equation for this distribution, introducing his famous bracket [2], and in a remarkable paper, which deserves to be better known, Baker [3] argued the converse, that the equation proposed by Moyal, together with a projection property of the Wigner distribution function, implied quantum mechanics. More than 25 years ago one of us (DBF) [4] wrote an article in which he attempted to motivate these equations of phase space quantum mechanics from probability arguments. The starting point was the postulate of the existence of a real function  $f(x, p, t)$ , the Wigner distribution, which acts as quasi-probability distribution function in the sense that the energy  $E$  of a system (taken as one-dimensional for simplicity of presentation) is the expectation value of the Hamiltonian  $H(x, p)$  of the system with respect to the real, but not necessarily positive, distribution  $f(x, p, t)$ . Symbolically;

$$E = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H(x, p) f(x, p, t) dx dp}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, p, t) dx dp}. \quad (1)$$

The idea of [4] was to describe a local relation between  $f$  and  $H$  such that this equation would be automatically true, upon integration, whatever choice of  $H(x, p)$  is made. He deduced from it two equations (6) which are easily seen to be a consequence of the time independent Schrödinger equation. To explain those equations, which are the starting point of this discussion it is most convenient to begin with the definition of  $f$  in terms of the Schrödinger wave function  $\psi(x, t)$

$$f(x, p, t) = \int_{-\infty}^{\infty} \bar{\psi}(x-y, t) \psi(x+y, t) \exp\left(\frac{2ipy}{\hbar}\right) dy. \quad (2)$$

Now suppose  $\psi(x, t)$  is expanded in terms of normalized time-independent eigenfunctions  $\psi_j(x)$  as

$$\psi(x, t) = \sum_j a_j \psi_j(x) e^{(i/\hbar)E_j t}. \quad (3)$$

Then, in terms of the functions  $f_{jk}$ , which are density matrix elements given by

$$f_{jk}(x, p) = \int_{-\infty}^{\infty} \bar{\psi}_j(x-y) \psi_k(x+y) \exp\left(\frac{2ipy}{\hbar}\right) dy \quad (4)$$

we have

$$f(x, p, t) = \sum_{j,k} a_j^* a_k f_{jk} e^{-i(\hbar)(E_j - E_k)t}. \quad (5)$$

In [4] it is shown that the  $f_{jk}$  satisfy two equations, which follow directly from the time-independent Schrödinger equation (note: the same method of proof is discussed below in the derivation of (31)):

$$\cos\{f_{jk}(x, p), H(x, p)\} = (E_j + E_k) f_{jk} \quad (6a)$$

$$\sin\{f_{jk}(x, p), H(x, p)\} = -i(E_j - E_k) f_{jk} \quad (6b)$$

where the cosine and the sine brackets are the even and  $-i \times$  odd powers of an expansion of the exponential bracket in powers of  $\hbar/2$

$\exp i\{f(x, p), g(x, p)\}$

$$\stackrel{\text{def}}{=} f(x, p) * g(x, p) \\ = \frac{2}{\pi^2 \hbar^2} \int \exp\left\{\frac{2i}{\hbar} \begin{vmatrix} 1 & 1 & 1 \\ x & x' & x'' \\ p & p' & p'' \end{vmatrix}\right\} f(x', p') g(x'', p'') dx' dx'' dp' dp'' \quad (7a)$$

$$= \lim_{\substack{x' \rightarrow x \\ p' \rightarrow p}} 2 \exp\left\{\frac{i\hbar}{2} \left(\frac{\partial^2}{\partial x \partial p'} - \frac{\partial^2}{\partial x' \partial p}\right)\right\} f(x, p) g(x', p'). \quad (7b)$$

The sine bracket is in fact just another name for the Moyal bracket, and equation (6b) is the time-independent formulation of the equation for the density matrix elements which is equivalent to the Schrödinger equation [2, 3]. Equation (6a) appears in reference [4] where it is explicitly verified for the case of the harmonic oscillator but has never to our knowledge been taken up elsewhere.

It is this equation (6a), the 'third equation' of the title, which is the focus of the present article, whose purpose it is to extend equations (6a, b) to the time-dependent case, guided by more recent understanding of the role of the exponential bracket as

the unique associative product [5-7] and of the supersymmetric nature of the algebra generated by the sine and cosine brackets, which is already implicit in the equations of Baker's paper [3]! These insights suggest that the exponential bracket, or star product, as it is alternatively called is the fundamental entity, and that corresponding to (6b), for which a time-dependent extension has been known from the beginning of the subject, a similar extension ought to exist for (6a). In order to produce this equation, we are led to the introduction of an additional variable, which we call  $s$ , which plays the role of the imaginary part of a complex time, but also appears by itself. We should emphasize at this point that since we can exhibit solutions of the new equation corresponding to any given quantum-mechanical eigenfunction expansion, this parameter  $s$  may just be an artifact, and the new equation just a consistency condition to be fulfilled. On the other hand, equations often have a life of their own, and admit solutions beyond their original region of validity. Some of these issues are examined in the last section, where the solution corresponding to a free particle is discussed.

## 2. Some useful identities

A number of identities on the sine and cosine brackets will be used throughout this paper. To display them it is convenient to revert to a notation similar to Baker's original one:

$$f * g \stackrel{\text{def}}{=} \exp i\{f, g\} \quad (8a)$$

$$(f, g) \stackrel{\text{def}}{=} \cos\{f, g\} \quad (8b)$$

$$[f, g] \stackrel{\text{def}}{=} \sin\{f, g\} \quad (8c)$$

$$f \cdot g \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, p, t) g(x, p, t) dx dp \quad (8d)$$

$$E^*(f) \stackrel{\text{def}}{=} 1 + f + \frac{1}{2!} f * f + \frac{1}{3!} f * f * f + \dots \quad (8f)$$

The star exponential  $E^*(f)$  is well-defined as the star product is associative. Note that:

$$f * g = (f, g) + i[f, g]. \quad (9)$$

The following identities hold:

$$[f, g] \cdot h = [h, f] \cdot g = [g, h] \cdot f \quad (10a)$$

$$(f, g) \cdot h = (h, f) \cdot g = (g, h) \cdot f \quad (10b)$$

$$[f, g] = -[g, f] \quad (10c)$$

$$(f, g) = (g, f) \quad (10d)$$

$$[[f, g], h] + [[h, f], g] + [[g, h], f] = 0 \quad (10e)$$

$$[(f, g), h] + [(h, f), g] + [(g, h), f] = 0 \quad (10f)$$

$$[(f, g), h] + [(h, f), g] + [(g, h), f] = 0. \quad (10g)$$

All these identities, with the exception of the last, are in Baker's paper [3], and are Jacobi identities for a superalgebra, though nobody realized it at the time! Those which are not obvious may be easily proved by going to a Fourier resolution for  $f, g, h$ .

The following identities will also be useful:

$$E^*(-f)*E^*(f) = E^*(f)*E^*(-f) = 1 \quad (11)$$

and

$$E^*(\lambda H)*f*E^*(-\lambda H) = \sum \frac{(-2i\lambda)^r}{r!} [\dots [[f, H], H] \dots, H] \quad (12a)$$

$$E^*(\lambda H)*f*E^*(\lambda H) = \sum \frac{(2\lambda)^r}{r!} (\dots ((f, H), H) \dots, H) \quad (12b)$$

(c.f. the identities familiar from exponentiation:

$$\exp(\lambda H)f \exp(-\lambda H) = \sum \frac{\lambda^r}{r!} [\dots [[f, H], H] \dots, H] \quad (13)$$

$$\exp(\lambda H)f \exp(\lambda H) = \sum \frac{\lambda^r}{r!} \{\dots \{f, H\}, H\} \dots, H\}$$

where the star product is identified with the ordinary product, the star exponential with the ordinary exponential, and  $2i$  times the sine bracket and  $2$  times the cosine bracket with the ordinary commutator  $[, ]$  and anticommutator  $\{, \}$ , respectively.) To prove (11), expand the star exponentials according to (8f), use associativity of the star product, and regroup. To prove (12), use a similar method, and regroup using

$$f*H - H*f = 2i[H, f] \quad f*H + H*f = 2(H, f) \quad (14)$$

which follow directly from (9). The factors of  $2$  and  $i$  on the right-hand side of (14) are the extra factors of  $2$  and  $i$  which appear in (12) compared with (13).

### 3. The time-dependent case

Baker [3] demonstrates that the two equations

$$\hbar \frac{\partial}{\partial t} f(x, p, t) = [f(x, p, t), H(x, p)] \quad (15)$$

$$(f(x, p, t), f(x, p, t)) = \alpha f(x, p, t) \quad (16)$$

where  $\alpha$  is a proportionality constant, are equivalent to the conventional formulation of time-dependent quantum mechanics. He shows that (16) implies the existence of a wavefunction  $\psi(x, t)$  such that  $f(x, p, t)$  may be expressed in the form (2), and that (15) then implies that  $\psi(x, t)$  satisfies the time-dependent Schrödinger equation. Equation (15) is just the well known Liouville equation for the Wigner function, and clearly gives (6b) when  $f(x, p, t)$  is expressed in terms of an eigenfunction expansion as in equation (5). Note that since the sine bracket is antisymmetric (16) may be written equally well in terms of the star product as

$$f(x, p, t)*f(x, p, t) = \alpha f(x, p, t). \quad (17)$$

It is easy to see that (16) is compatible with (15). By this we mean that if  $f$  satisfies (15), then so does  $(f, f)$

$$[[f, f], H] = 2([f, H], f) = 2 \left( \hbar \frac{\partial}{\partial t} f, f \right) = \hbar \frac{\partial}{\partial t} (f, f) \quad (18)$$

where we have used (10f) in the first equality and (15) in the second.

#### 4. A further generalization

The problem remains as to how to extend equation (6a) so that it will continue to hold in the time-dependent case. An obvious generalization would be to extend the functional dependence of  $f$  to an additional variable,  $s$  say, and postulate the equations

$$\hbar \frac{\partial}{\partial s} f(x, p, s, t) = (f(x, p, s, t), H(x, p)) \quad (19a)$$

$$\hbar \frac{\partial}{\partial t} f(x, p, s, t) = [f(x, p, s, t), H(x, p)]. \quad (19b)$$

With an eigenfunction expansion for  $f(x, p, s, t)$  of the form

$$f(x, p, s, t) = \sum_{j,k} a_j^* a_k f_{jk} \exp\left(-\frac{i}{\hbar} (E_j(t+is) - E_k(t-is))\right) \quad (20)$$

it is evident that equations (19) reproduce (6).

Equation (19a) is a new equation. It is interesting to note that if both (19a) and (19b) are to be satisfied simultaneously, then an integrability condition arising from the two ways of evaluating  $[\partial^2 f(x, p, s, t)]/\partial s \partial t$  must be fulfilled. In fact it is always satisfied in consequence of the identity  $[(f, H), H] = [(f, H), H]$ , which is a special case of (10f).

However, the nonlinear relation (16) is not compatible with (19a), nor does the eigenfunction expansion (20), which gives the time-independent equation (6a), satisfy (16), as there is no  $s$ -dependence yet. Is it possible to modify (16) in such a way that *compatibility of all three equations is maintained and there is no conflict with orthodox  $s$ -independent quantum mechanics?* It turns out that in fact (16) requires very little modification, beyond the replacement of  $t$  by  $t-is$ . In a manner which we shall explain (16) can be viewed as a boundary condition.

First we introduce the following modification; postulate an  $f(x, p, s, t)$  such that

$$f(x, p, s, t) * f(x, p, -s, t) = \alpha f(x, p, 0, t-is). \quad (21)$$

It is easy to verify that the expansion (20) satisfies (21), provided the following orthonormality conditions on the time-independent density matrix elements are fulfilled:

$$f_{uj} * f_{kl} = \delta_{jk} f_{il}. \quad (22)$$

These are the same orthonormality conditions that occur in the  $s$ -independent case [4]. As in (18), the compatibility of (21) with (19b) is a consequence of (10). Compatibility with (19a) is proved as follows. Differentiate (21) with respect to  $s$ ;

$$\begin{aligned} \alpha \hbar \frac{\partial}{\partial s} f(x, p, 0, t-is) &= \hbar \frac{\partial}{\partial s} f(x, p, s, t) * f(x, p, -s, t) + \hbar f(x, p, s, t) * \frac{\partial}{\partial s} f(x, p, -s, t) \\ &= (f(x, p, s, t), H) * f(x, p, -s, t) - f(x, p, s, t) * (H, f(x, p, -s, t)) \\ &= -i[f(x, p, s, t), H] * f(x, p, -s, t) + i f(x, p, s, t) * [H, f(x, p, -s, t)] \\ &= -i \alpha \hbar \frac{\partial}{\partial t} f(x, p, 0, t-is). \end{aligned} \quad (23)$$

But this is an identity on account of the independence of  $f(x, p, 0, t - is)$  upon  $t + is$ . The third line in the above derivation follows from the second since  $f * H = (f, H) + i[f, H]$  is an associative product, so that there is a cancellation of terms.

The next step is to manipulate (16) to cast it in the form of equation (21). Write (16) with the argument shifted to  $t - is$ ;

$$f(x, p, 0, t - is) * f(x, p, 0, t - is) = \alpha f(x, p, 0, t - is). \tag{24}$$

The remarkable fact is that the left-hand side of this equation together with (19a, b) implies the left-hand side of (21). Expand the left-hand side of (24) in a Taylor expansion in  $s$ ;

$$\begin{aligned} & f(x, p, 0, t - is) * f(x, p, 0, t - is) \\ &= \sum \frac{(-is)^m}{m!} \frac{\partial^m f(x, p, 0, t)}{\partial t^m} * \sum \frac{(-is)^n}{n!} \frac{\partial^n f(x, p, 0, t)}{\partial t^n}. \end{aligned} \tag{25}$$

Now convert to sine brackets:

$$\begin{aligned} &= \sum \frac{s^m [\dots [[f(x, p, 0, t), H], H], \dots H]}{(i\hbar)^m m!} \\ &* \sum \frac{s^n [\dots [[f(x, p, 0, t), H], H], \dots H]}{(i\hbar)^n n!}. \end{aligned} \tag{26}$$

Use (12a), (11), and (12b) to convert the sine brackets in the above expansion into cosine brackets:

$$\begin{aligned} &= \sum \frac{s^m (\dots ((f(x, p, 0, t), H), H), \dots H)}{\hbar^m m!} \\ &* \sum \frac{(-s)^n (\dots ((f(x, p, 0, t), H), H), \dots H)}{\hbar^n n!}. \end{aligned} \tag{27}$$

Next, the nested cosine brackets are turned into derivatives with respect to  $s$  to give

$$= \sum \frac{s^m f^m(x, p, 0, t)}{m!} * \sum \frac{(-s)^n f^n(x, p, 0, t)}{n!}. \tag{28}$$

(Here  $f^n(x, p, 0, t)$  denotes  $(\partial^n / \partial s^n) f(x, p, s, t)|_{s=0}$ .) But this expression is just the Maclaurin expansion of the left-hand side of (21),

$$= f(x, p, s, t) * f(x, p, -s, t) = \alpha f(x, p, 0, t - is) \tag{29}$$

where the last equality uses (24). Thus (16) is in the nature of a boundary condition upon  $f(x, p, s, t - is)$  where the third variable is set to zero.

**5. Interpretation**

Two views are possible. The conservative approach is that equations (19) and (21) in fact add nothing to the physics of the situation, as a solution  $f(x, p, s, t)$  to those equations can always be built from a conventional quantum-mechanical wavefunction by way of an eigenfunction expansion and substitution in (20). Thus the role of the additional parameter  $s$  is entirely spurious.

The unconventional point of view would be to trust the equations, and ask whether they admit solutions, which though perhaps representable in terms of an eigenfunction expansion, surpass the familiar description of quantum-mechanical events, and possibly cast some light on the measurement process. A central issue is whether there exists some sort of physical interpretation for the parameter  $s$ . In some respects it behaves like an inverse negative temperature, as the classical solution of (19), (21), i.e. in the limit  $\hbar \rightarrow 0$ , is, for time-independent Hamiltonians, simply  $f(x, p, s) = \alpha \exp(2H(x, p)s)$ , reminiscent of the Boltzmann distribution. Another possibility is that the physics of the situation for a one-particle system, evolving in a two-dimensional phase space is best described in a four-dimensional manifold, according to equations (19) and (21). However, it may be that only the subspace  $x, p, t$  is physically accessible to us, and we can only perceive objects at  $s = 0$ .

Further insight into the nature of the variable  $s$  comes from recasting the theory with the additional  $s$  variable in terms of a wavefunction  $\psi(x, s, t)$ , which is related to  $f(x, p, s, t)$  by a construction similar to (2), as indeed is guaranteed by (24) and the results of Baker [3]. Then, just as (19b) is equivalent to the Schrödinger equation

$$-i\hbar \frac{\partial}{\partial t} \psi(x, s, t) = H(x, p)\psi(x, s, t) \quad (30)$$

then the cosine bracket equation (19a) is equivalent to

$$\hbar \frac{\partial}{\partial s} \psi(x, s, t) = H(x, p)\psi(x, s, t). \quad (31)$$

On the right-hand sides of these equations  $H$ , of course, is to be interpreted as an operator. These equations are consistent with the hypothesis that the dependence of  $\psi$  upon  $s, t$  is through the single complex variable  $z = t - is$ . Note that it is only  $\psi$  which has this simple behaviour;  $f$  depends upon both  $z$  and  $\bar{z}$ . This observation lends support to the conservative viewpoint that (19a) is merely a construct, and has no greater significance.

As further verification, we show that (30) and (31) imply (19a, b). Consider:

$$\begin{aligned} f^*H &= \frac{2}{\pi^2 \hbar^2} \int \exp \left\{ \frac{2i}{\hbar} \begin{vmatrix} 1 & 1 & 1 \\ x & x' & x'' \\ p & p' & p'' \end{vmatrix} \right\} \bar{\psi}(x' - y, s, t) \psi(x' + y, s, t) \exp \left( \frac{2ip'y}{\hbar} \right) \\ &H(x'', p'') dx' dx'' dp' dp'' dy \\ &= \frac{2}{\pi \hbar} \int \exp \left( \frac{2ip}{\hbar} (x + y - x') + \frac{2ip''}{\hbar} (x' - x) \right) \bar{\psi}(x' - y, s, t) H(x + y, p'') \\ &\quad \times \psi(x' + y, s, t) dx' dp'' dy \\ &= \frac{2}{\pi \hbar} \int \exp \left( -\frac{2ip}{\hbar} u + \frac{2ip''}{\hbar} (u + v - x) \right) \bar{\psi}(x + u, s, t) H(v, p'') \\ &\quad \times \psi(2v + u - x, s, t) du dp'' dv \\ &= 2 \int \exp \left( -\frac{2ip}{\hbar} u \right) \bar{\psi}(x + u, s, t) H \left( x - u, -\frac{\hbar}{i} \frac{\partial}{\partial(x - u)} \right) \\ &\quad \times \psi(x - u, s, t) du \end{aligned} \quad (32)$$



where the substitutions  $u = x' - v$  and  $v = x + y$  have been introduced. The last line follows from the penultimate by consideration of the integral

$$\int \exp\left(\frac{2ip''}{\hbar}(u+v-x)\right) H(v, p'') \psi(2v+u-x, s, t) dp'' dv$$

$$= \pi \hbar H\left(v, -\frac{\hbar}{i} \frac{\partial}{\partial v}\right) \psi(v, s, t)|_{(x-u)}. \quad (33)$$

$H(v, p'')$  is assumed expanded in a power series in  $p''$  before integration. If  $H(x, p)$  separates into a kinetic term plus a  $p$  independent term the result follows directly. If not, then  $H(x, -(\hbar/i)(\partial/\partial x))$  must be interpreted as a normal ordered operator in the usual way. In a similar fashion

$$\overline{f^*H} = \int \exp\left(-\frac{2ip}{\hbar}u\right) \psi(x-u, s, t) H\left(x+u, +\frac{\hbar}{i} \frac{\partial}{\partial(x+u)}\right) \bar{\psi}(x+u, s, t) du. \quad (34)$$

Then taking (32)  $\pm$  (34) and using (30) and (31), we obtain (19a, b) as claimed.

## 6. The free particle

Suppose  $H = p^2/2m$ , then from (7b) we see that (19a, b) become

$$\frac{\partial f}{\partial s} = \frac{p^2}{\hbar m} f - \frac{\hbar}{4m} \frac{\partial^2 f}{\partial x^2} \quad (35a)$$

$$\frac{\partial f}{\partial t} = \frac{p}{m} \frac{\partial f}{\partial x}. \quad (35b)$$

Equation (35b) is satisfied by following functional dependence upon  $x, p, t$ :

$$f(x, p, s, t) = f\left(x + \frac{p}{m}t, p, s\right). \quad (36)$$

Using an integrating factor then (35a) becomes just the heat equation for

$$g\left(x + \frac{p}{m}t, p, s\right) = e^{-p^2 s / \hbar m} f\left(x + \frac{p}{m}t, p, s\right) \quad (37)$$

$$\frac{\partial g}{\partial s} = -\frac{\hbar}{4m} \frac{\partial^2 g}{\partial x^2}. \quad (38)$$

Now from (7b) it is easy to see that the star product in the boundary condition (24) becomes the ordinary product

$$f(x, p, 0, t-is)f(x, p, 0, t+is) = \alpha f(x, p, 0, t-is). \quad (39)$$

Hence  $f$  must be either 0 or  $\alpha$ , i.e. a linear combination of theta functions, with alternating coefficients  $\pm\alpha$ .

The heat equation possesses an elementary solution of Gaussian form:

$$g = \frac{1}{\sqrt{-2\pi s}} \exp\left(\frac{m(x + (p/m)t)^2}{\hbar s}\right). \quad (40)$$

Note that as  $s \rightarrow 0$  from below this approaches a delta function. It does not, however, satisfy (39); but remembering that in consequence of the linearity of (19a) any linear functional of a solution is also a solution, provided all operators introduced commute with the derivatives we can find a solution in the form of an error function

$$f(x, p, s, t) = \alpha \frac{\exp(sp^2/\hbar m)}{\sqrt{-2\pi s}} \int_{-\infty}^{(x+(p/m)t)} \exp(mu^2/\hbar s) du. \quad (41)$$

As  $s \rightarrow 0$  from below, the distribution function  $f$  approaches a theta function of  $(x + pt/m)$  and hence satisfies (39). The general solution for  $f(x, p, s, t)$  will therefore be expressible as a similar linear combination of error functions. It is interesting to note that Bartlett and Moyal discussed the distribution function for a free particle in 1949 [8].

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